Approximations for Coulomb Barrier Transmission Probability in HETC and Related Codes

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Abstract

A number of methods are discussed for approximating an s-wave Coulomb barrier transmission probability. The methods are designed for computational efficiency, and have been implemented as a Fortran subroutine library for applications in INCA, FBRK, and HETC Monte Carlo codes.

Introduction

In the HETC code, the effect of a Coulomb barrier must be considered at three stages in the computational scheme.

1. The probability that a charged particle incident on a nucleus will interact is modified by the presence of a Coulomb barrier.
2. A charged particle attempting to escape the nucleus during the intranuclear cascade must pass the Coulomb barrier.
3. During the subsequent evaporation (or Fermi breakup) phase, the emission probability for a charged particle is reduced by the Coulomb barrier.

The present study is directed toward items 1 and 3 with respect to a repulsive Coulomb potential; the effect of an attractive Coulomb potential (i.e. incident π^- or $\bar{p}$) is not treated.

Up to the present time, HETC (and the intranuclear cascade codes VEGAS and ISABEL) have ignored the effect of the Coulomb barrier on the interaction of a charged particle with a target nucleus. The INCA intranuclear cascade code

[1] approximates an effective cross section σ_{eff} for charged particle interactions by

$$\sigma_{eff} = \sigma_g T_c(\epsilon)$$

where σ_g is the geometric cross section, ϵ is the kinetic energy in the center of mass, E_c is the Coulomb energy at an appropriate nuclear radius, and $T_c(\epsilon)$ is a barrier transmission probability given by

$$T_c(\epsilon) = \begin{cases} 1 - E_c/\epsilon & \text{for } \epsilon > E_c \\ 0 & \text{for } \epsilon \leq E_c \end{cases} \tag{1}$$

The transmission probability of equation 1 is just the probability of interaction for charged particles incident uniformly on a disk σ_g which may be derived from classical orbit theory for repelling charges. It vanishes at the Coulomb barrier and allows no probability of penetration.

For charged particles attempting to leave the nucleus during the intranuclear cascade, those with energy below the barrier are trapped while those above are either emitted totally or reflected/refracted with a probability which considers the Coulomb barrier. The present study does not address this area.

In the traditional implementation of the evaporation model [2], as is used in HETC and in many evaporation codes, a barrier transmission probabilty is assumed with the form

$$T(\epsilon; k) = \begin{cases} 1 - kE_c/\epsilon & \text{for } \epsilon > kE_c \\ 0 & \text{for } \epsilon \leq kE_c \end{cases} \tag{2}$$

where $k < 1$ reflects the effect of barrier penetration. The form of equation 2 is desirable from the standpoint of computational efficiency; as we shall see below, it may be quite a reasonable approximation in some cases. However, in the implementation of the evaporation model, equation 2 appears only as a factor in a integrand in the computation of the charged particle emission probabilities and so it is the choice of the parameter k that is relevant.

In the FBRK Fermi breakup code (INCA2 in reference [1]), the breakup channel probabilty includes a factor which is an approximate fit to the nonrelativistic *s-wave* Coulomb barrier transmission probability (with an additional probability factor for higher angular momenta). This fit was noticeably inaccurate at energies just below the Coulomb energy for light nuclei, providing a major motivation for this study. In addition, the use of such an s-wave approximation may provide the most reasonable lowest order correction for barrier transmission for the incident particle described as item 1 above.

S-wave Transmission Probability

A general description of methods for calculating the nonrelativistic Coulomb wave functions $F_L(\rho, \eta)$ and $G_L(\rho, \eta)$ for arbitrary angular momentum L may be found in references [3] and [4]. The variables ρ and η are be defined by

$$\begin{aligned}\rho &= \hbar^{-1}(R_1 + R_2)\sqrt{2\mu\epsilon} \\ \eta &= \hbar^{-1} Z_1 Z_2 e^2 \sqrt{\mu/2\epsilon}\end{aligned}$$

where Z_1, Z_2 are the charge numbers of the two particles, R_1, R_2 are appropriately chosen Coulomb radii for the particles, μ is the reduced mass of the two particle system, and ϵ is the kinetic energy in the center of mass. The use of nonrelativistic Coulomb wave functions to obtain the transmission probability is justified since the transmission probability approaches unity when relativistic effects become significant, and little error may be introduced.

The objective of this work is to provide algorithms which approximate the s-wave transmission probability accurately and with reasonable efficiency. The s-wave transmission probability is given by

$$T_0(\rho,\eta) = \frac{1}{F_0(\rho,\eta)^2 + G_0(\rho,\eta)^2}$$

where F_0 and G_0 are the s-wave Coulomb wave functions. The fit is required to match at $\rho = 2\eta$, i.e. at the Coulomb barrier, and to have the limits

$$\begin{aligned}\lim_{\rho\to 0} T_0(\rho,\eta) &= \frac{2\pi\eta}{e^{2\pi\eta} - 1} = C_0(\eta) \\ \lim_{\rho\to\infty} T_0(\rho,\eta) &= 1\end{aligned}$$

With considerable guidance from the various approximations and asymptotic forms discussed in [4], the fitting procedure was carried out largely by trial and error.

In the discussion following, it is frequently convenient to treat T_0 as a function of the variables ξ and x, rather than ρ and η, where

$$\xi = 2\rho\eta = 4Z_1 Z_2 (R_1 + R_2) e^2 \mu/\hbar^2$$

and

$$x = \frac{\rho}{2\eta} = \frac{(R_1 + R_2)\epsilon}{Z_1 Z_2 e^2} = \frac{\epsilon}{E_c}$$

The variable ξ is independent of energy and is a constant for any projectile-target pair. The value of ξ varies from $\xi \approx 0.015$ for $\pi^+ + {}^2\mathrm{H}$ to $\xi \approx 10^6$ for ${}^{238}\mathrm{U} + {}^{238}\mathrm{U}$. Approximations for large ξ are included in the present work for use with heavy ion projectiles in the ISABEL code and for the future extension of HETC to heavy ion transport.

The various techniques discussed below provide a complete prescription for obtaining T_0 for $\xi \leq 10000$ and for all x, although in most Monte Carlo applications probabilities $< 10^{-6}$ may be considered negligible. For $\xi > 10000$

(heavy nucleus-nucleus collisions), only the range of energies from just below the Coulomb barrier is treated accurately; the transmission probability vanishes so rapidly below the barrier that for most potential applications the approximation is probably sufficient, although the methods described below could be extended to higher ξ if the need arises in the future.

In developing and testing the methods described below, use has been made of a subroutine which does an "exact" calculation of the Coulomb wave functions $F_L(\rho,\eta)$ and $G_L(\rho,\eta)$ for arbitrary order L. For very large ξ and small x, excessive computing time has prevented an exact calculation for testing purposes; however, in these cases, the transmission probability T_0 is less than 10^{-100}.

Approximation Methods

Approximation for $x > 1$

For the region $\epsilon \geq E_c$ ($x \geq 1$) and for all ξ, a convenient approximation may be derived from the formulae of reference [4]. In this region, we may use

$$T_0(\rho,\eta) \approx \sqrt{1.0 - \frac{2\eta^{7/6}}{0.11225 + 0.5\eta^{1/2} + \rho\eta^{1/6}}} \tag{3}$$

Equation 3 is accurate to about $\pm 12\%$ over the entire range of ξ. It is very accurate at $x = 1$, with the maximum error occuring just above the Coulomb energy for large ξ. The transmission probability is underestimated for low ξ and overestimated for large ξ. In view of the utility of the approximation (3), the obtainable accuracy was taken as the upper limit for the allowed error in estimating the transmission probability below the Coulomb energy.

It was observed that for a small range in ξ the simple approximation from equation 2, in the form

$$T_0(\rho,\eta) \approx 1 - [1 - T_0(2\eta,\eta)]\frac{2\eta}{\rho} \tag{4}$$

has a smaller maximum error than (3); consequently it is used in that range, with a table lookup method employed to evaluate $T_0(2\eta,\eta)$.

Table Lookup Range $0.0316 \leq \xi \leq 10000$

For energies less than but comparable to the Coulomb energy ($0.1 < x < 1$), it is very difficult to find a single mathematical approximation that satifies the requirements. Therefore, to treat this region, a table lookup procedure was adopted. For $0.031623 \leq \xi \leq 316.23$ and $0.1 \leq x \leq 1$, the quantity $\ln T_0$ is tabulated on an 81×21 logarithmic grid in ξ and x, twenty points per decade in both variables. A second tabulation on a 61×61 logarithmic grid in ξ and x is used for the range $316.23 \le \xi \le 10000$ for $0.031623 \le x \le 1$, forty points per decade in both variables. With these grids, the accuracy is generally a few percent, with some observed errors as large as 15% at large ξ and $x \approx 1$. The range covered by this method is sufficient to treat $^{40}\mathrm{Ca} + {}^{40}\mathrm{Ca}$.

Approximation for $0.0316 \le \xi \le 10000$

At all values of x which are below the range of the tabulations ($x < 0.1$ or $x < 0.0316$), the following approximation was developed by empirical methods. It may be shown, from integral representations of the Coulomb wave functons [4],that

$$\lim_{x\to 0} \frac{C_0(\eta)}{T_0} = f_0^2(\xi)$$

where

$$f_0(\xi) = \int_0^\infty e^{-(y+\xi/y)}\, dy$$

Applying the empirically derived correction terms, the approximation is

$$T_0 \approx \frac{C_0(\eta)}{[f_0(\xi)(1 + x/3 + 0.3x\sqrt{\xi} + 0.1x^2\xi)]^2} \tag{5}$$

where the value of $f_0(\xi)$ is precalculated and obtained by a table lookup method. The accuracy of equation 5 is better, and generally much better, than 5% over the specified range of ξ and x.

Approximation for Very Small ξ

For very low values of ξ ($\xi < 0.031623$), the approximation for T_0 is obtained from a low order expansion of F_0 and G_0 in reference [4]. Let

$$\begin{aligned}
t_1 &= (1 - 3\xi^2/4 + 5x\xi^2)\cos\rho - (\xi\rho/2)\sin\rho \\
t_2 &= 1 + \xi(1 - x/6)/2 \\
t_3 &= \log\xi + 2\gamma - 1 + 1/12\eta^2 + 1/120\eta^4 \text{ for } \eta > 1 \\
&= \log 2\rho + \gamma - 1/(1+\eta^2) + 0.2020569\eta^2 + 0.08232323\eta^4 \text{ for } \eta \le 1
\end{aligned}$$

where

$$\gamma = 0.5772157...$$

Then for

$$\begin{aligned}
t_G &= t_1 + \xi t_2 t_3 \\
t_F &= C_0(\eta)\rho t_2
\end{aligned}$$

we obtain

$$T_0 \approx \frac{C_0(\eta)}{t_G^2 + t_F^2} \tag{6}$$

Equation 6 has an accuracy better than 1% over its range and could be used for somewhat larger ξ to reduce the size of the lookup tables. It is included primarily for completeness; for HETC, it is applicable only for π^+ on hydrogen isotopes.

Approximation for $\xi > 10000$ and $x < 1$

At the present time, the range $\xi > 10000$ and $x < 1$, which is appropriate for the collision of very heavy ions at energies below the Coulomb energy, is only roughly treated for completeness. The approximation consists in expressing

$$T_0(\rho, \eta) \approx T_0(2\eta, \eta)(\rho/2\eta)^{\alpha} \tag{7}$$

where $T_0(2\eta, \eta)$ is obtained from equation 3 and

$$\alpha = \frac{2\eta^{7/3}}{(0.11225 + 0.5\eta^{1/2})(0.11225 + 0.5\eta^{1/2} + 2\eta^{7/6})}$$

is obtained by matching the slope of equation 7 to the slope of equation 3 at $\rho = 2\eta$. Equation 7 is reasonably accurate only down to transmission probabilities of about 1%.

Conclusions

The code developed in this effort consists of routines for generating the necessary tables and parameters, routines for reading and writing the data tables, and the function subprograms which calculate the nonrelativistic s-wave transmission probability exactly, in the general approximation scheme, and in the simple approximation of equation 4. Conclusions with respect to the accuracy of the methods developed were obtained by extensive comparison of the approximation with the exact calculation of the transmission probabity both as a function of ρ and η and for particular combinations of projectile and target nucleus. The overall accuracy may be considered as 12%, with isolated discrepancies as large as 15% being noted at boundaries between ranges corresponding to different approximation schemes. At both low and high energies for $\xi \leq 10000$, the accuracy is generally much higher.

In figures 1 through 4, exact and approximate calculations for the transmission probability are illustrated. In all four examples, the results of the full approximation (dotted line) are nearly coincident with the exact calculation (solid line) below the Coulomb energy (vertical dotted line). In figure 2, the general approximation and the simple approximation of equation 4 are identical; in figure 1, they nearly coincide. However, the limitations of the simple approximation are readily apparent in figures 3 and 4; figure 3 is roughly the most extreme case in which the methodolgy of equation 4 is used implicitly in the evaporation model in HETC.

In the INCA intranuclear cascade code, the transmission probability must only be calculated once in each problem; it is then applied as a factor multipling the geometric cross section to estimate the effect of Coulomb repulsion on the interaction of projectile and target. Therefore the exact calculation has been implemented since execution time is not adversely affected.

For the FBRK Fermi breakup code, the general approximation scheme has been implemented to obtain the effect of the Coulomb barrier on the two-body breakup channels. However, since FBRK is applicable only to light nuclei, the data tables have been trucated to cover only the required range and have been added to the FBRK nuclear data file.

For HETC, the general approximation scheme has been implemented for the effect of Coulomb repulsion on the interaction of projectile and target, and the required data has been incorporated into the HETC data file. At each charged particle collision, the transmission probability obtained is used as the probability for allowing the nuclear interaction to occur; if disallowed, the potential particle interaction is rejected and the transport of the particle is continued. The general approximation method will also be implemented as part of the FBRK subroutines which will be inserted into HETC to supplement the evaporation model. In addition, the parameter $T_0(2\eta, \eta)$ is provided for use in future modifications to the evaporation model.

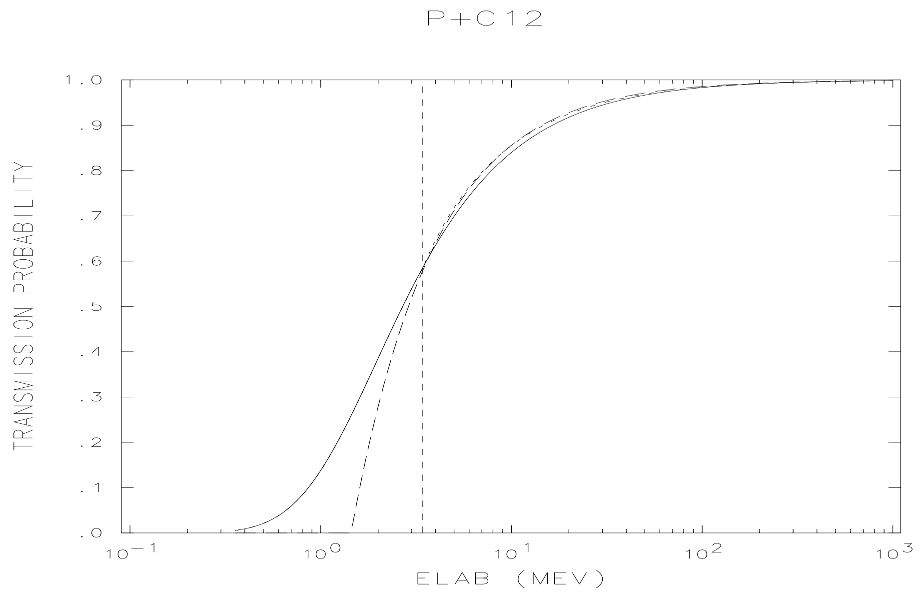

Figure 1: Transmission probability for p on ^{12}C. Solid line – exact calculation; dotted line – general approximation; dashed line – simple approximation.

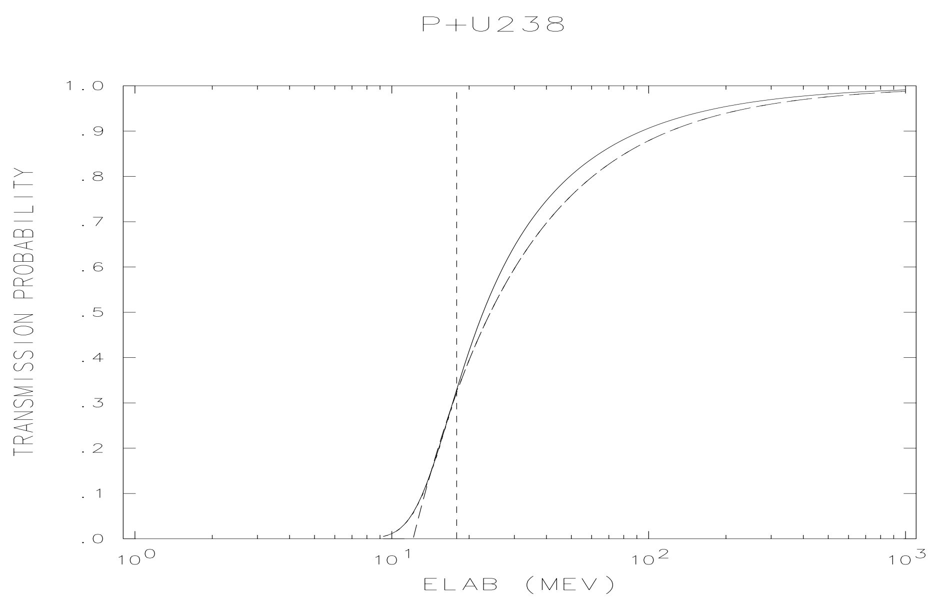

Figure 2: Transmission probability for p on ^{238}U. Solid line – exact calculation; dotted line and dashed line – general approximation and simple approximation (which coincide above the Coulomb energy).

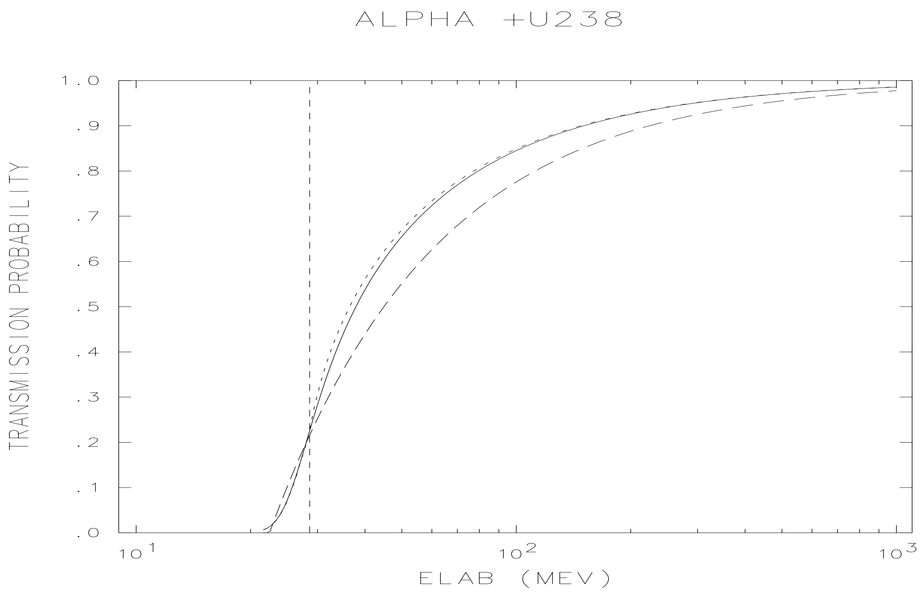

Figure 3: Transmission probability for α on ^{238}U. Solid line – exact calculation; dotted line – general approximation; dashed line – simple approximation.

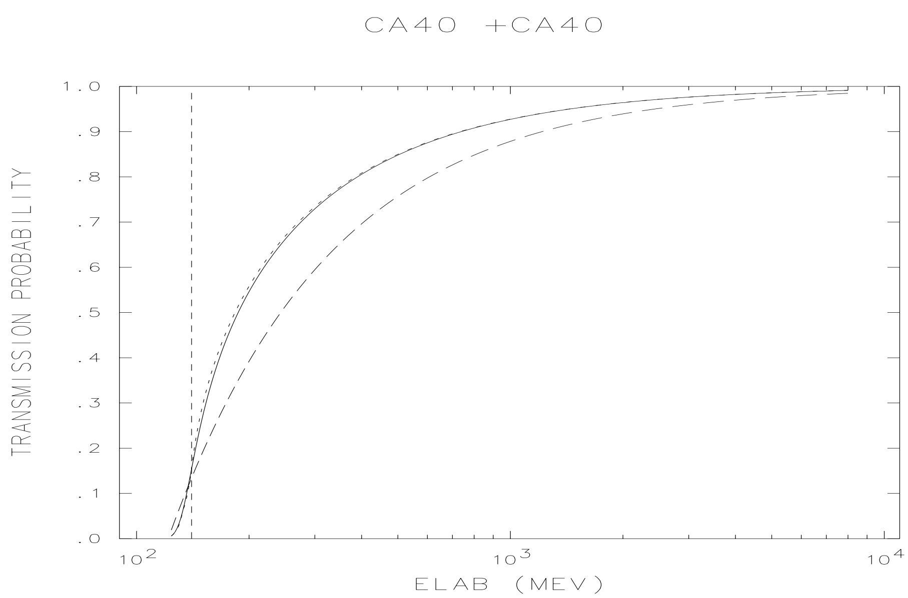

Figure 4: Transmission probability for ^{40}Ca on ^{40}Ca. Solid line – exact calculation; dotted line – general approximation; dashed line – simple approximation.

References

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